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(YIP) Robust Manipulation and Computation for Inhomogeneous Quantum Ensembles

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Washington University

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14. ABSTRACT

This project focused on the development of a novel control-theoretic framework with a set of tractable computational methods for robust manipulation of inhomogeneous quantum ensembles. Engineering the time evolution of quantum ensembles in a desired manner by using electromagnetic pulses of appropriate shape and frequency is an indispensable step that enables many applications in quantum control, such as nuclear magnetic resonance (NMR) spectroscopy and imaging, laser cooling, solid state physics, and quantum computation. This project carried out a fundamental investigation of ensemble control systems. New methods were established to analyze controllability of quantum ensembles through polynomial approximations, which inspired the development of a unified computational method based on pseudospectral approximations for solving optimal ensemble control problems. This newly developed computational method has been used to design optimal pulses for protein NMR spectroscopy, which have been experimentally implemented yielding a significant sensitivity enhancement over the conventional pulses. The scope of this project w

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Abstract

This project focused on the development of a novel control-theoretic framework with a set of tractable computational methods for robust manipulation and optimal control of inhomogeneous quantum ensembles. Engineering the time evolution of quantum ensembles in a desired manner by using electromagnetic pulses of appropriate shape and frequency is an indispensable step that enables many applications in quantum control, such as nuclear magnetic resonance (NMR) spectroscopy and imaging (MRI), laser cooling, solid state physics, quantum computation, and quantum information processing. This project carried out a fundamental investigation of ensemble control systems. New methods based on geometric control theory were established to analyze controllability of quantum ensembles through polynomial approximations, which inspired the development of a unified computational method based on pseudospectral approximations for solving optimal ensemble control problems. This newly developed computational method has been used to design optimal pulses for protein NMR spectroscopy, which have been experimentally implemented yielding a significant sensitivity enhancement over the conventional pulses. The scope of this project was extended beyond the control of quantum ensembles to general ensemble systems, where controllability characterization for linear and nonlinear ensemble systems was provided, and efficient optimization-free computational methods for optimal control synthesis for such systems were developed.

Accomplishments and New Findings

The objective of this project is to carry out a fundamental investigation of ensemble control problems involving the guidance of a large number or a continuum of structurally similar dynamical systems by the use of a common open-loop control. This class of problems originates from the study of the complex dynamics of large-scale quantum systems [1, 2, 3]. The novel achievements made through this funding support lead to further theoretical and practical developments in control theory with broad impact on the advancement of state-of-the-art quantum technologies.

Fifteen journal [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18] and thirteen peer-reviewed conference [19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31] papers have been published through the funding support period. Our research is multidisciplinary, and these papers appear in leading scientific journals and international conference proceedings across several disciplines including control theory and engineering, applied mathematics, physics, and bioengineering. The significant achievements and new findings through the support of this AFOSR YIP funding are summarized below.

1 Controllability of Ensemble Systems

We have extended the notion of ensemble controllability constructed in our previous work on quantum systems [3, 32] to general linear and nonlinear ensemble systems described below.

1.1 Finite-Dimensional Time-Varying Linear Ensemble Systems

We derived the necessary and sufficient controllability conditions for an ensemble of finite-dimensional time-varying linear systems indexed by a parameter β varying over a compact set K, given by

$$\frac{d}{dt}X(t,\beta) = A(t,\beta)X(t,\beta) + B(t,\beta)u(t), \quad \beta \in K \subset \mathbb{R}, \tag{1}$$

where the state is $X \in M \subset \mathbb{R}^n$, and $A \in L_\infty^{n\times n}(D)$ and $B \in L_2^{n\times m}(D)$ are $n \times n$ and $n \times m$ matrices, respectively, whose elements are complex-valued L_∞ and L_2 functions defined on a compact set $D = [0,T] \times K \subset \mathbb{R}^2$. The ensemble is controlled by the open-loop input $u \in L_2^m[0,T]$. We derived a Fredholm integral equation defined by the input-to-state operator that characterizes the dynamics of the ensemble, given by

$$(Lu)(\beta) = \int_0^T \Phi(0,\sigma,\beta)B(\sigma,\beta)u(\sigma)d\sigma = \xi(\beta), \tag{2}$$

where $\Phi(t,0,\beta)$ is the transition matrix for the inhomogeneous system $\dot{X}(t,\beta) = A(t,\beta)X(t,\beta)$, $\xi(\beta) = \Phi(0,T,\beta)X_F(\beta) - X_0(\beta)$, and $X_0(\beta)$ and $X_F(\beta)$ are the prescribed initial and terminal states. We showed that controllability of the ensemble system (1) is related to the singular system of the compact operator L as in (2), and is characterized by its singular values and singular functions [7]. We also derived an accompanying optimal ensemble control law as an infinite sum of weighted eigenfunctions of the operator L [7].

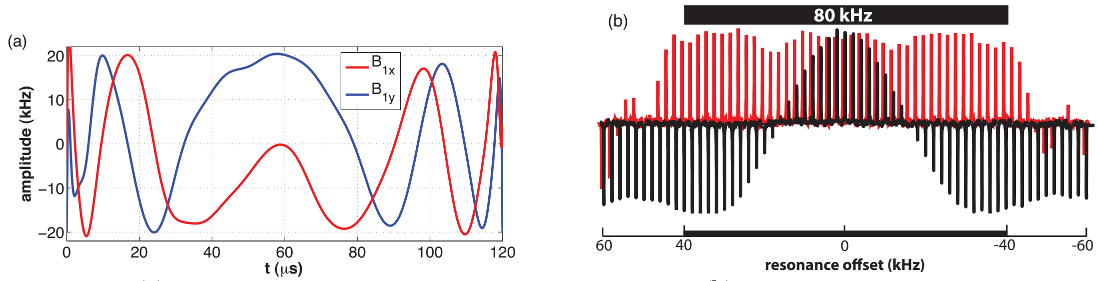
1.2 Nonlinear Ensemble Systems

The dynamics of a (weakly forced) nonlinear oscillator can be described by the phase-reduced model, $\dot{\theta} = f(\theta) + Z(\theta)u(t)$, where θ is the phase variable, f represents the system's baseline dynamics, Z is known as the phase response curve (PRC), and $u \in \mathcal{U} \subset \mathbb{R}$ is the external stimulus [33]. Phase models are widely employed in physics, chemistry, and biology [34] to study rhythmic systems where the oscillatory phase, but not the full state, can be observed, and where the PRC can be obtained experimentally. Employing tools from geometric control theory, we have analyzed the controllability of an ensemble of isolated nonlinear oscillators described by $\dot{\theta}_i = f_i(\theta_i) + Z_i(\theta_i)u(t)$, $i = 1, \ldots, N$, where f_i and Z_i are real-valued functions and $u \in \mathbb{R}$ [19, 16]. We showed that controllability is determined by the periodicity, or recurrence, of f_i and then by $\{f, \mathcal{Z}\}_{LA}$, that is, the Lie algebra generated by $f = (f_1, \ldots, f_N)'$ and $\mathcal{Z} = (Z_1, \ldots, Z_N)'$.

2 Computational Optimal Ensemble Control

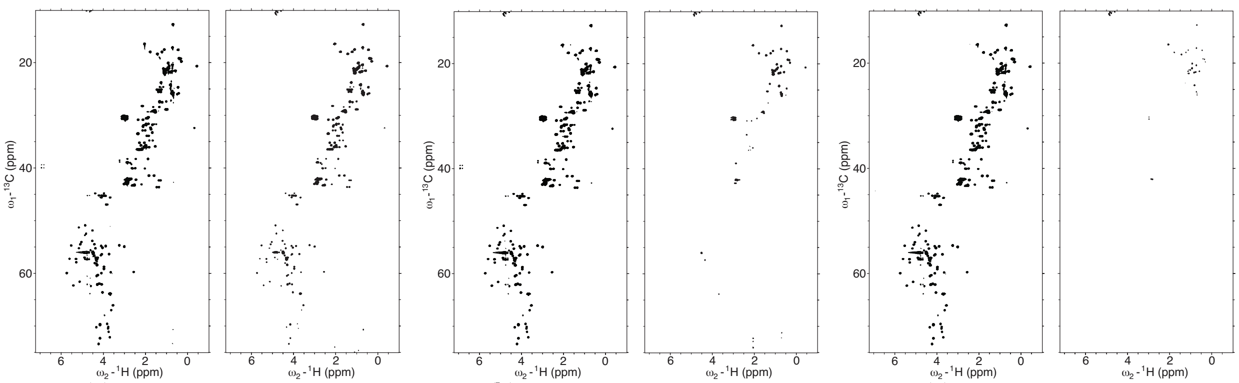
2.1 A Unified Computational Method for Optimal Pulse Design in Quantum Control

Designing an external field (a pulse sequence) that guides a quantum ensemble from an initial state to a desired target state in an optimal manner is a fundamental step in many applications in quantum control. Analytical solutions to such an optimal ensemble control problem are in general arduous to obtain or entirely unavailable, with the exception of a few special cases. Inspired by the method of converting an ensemble control problem to a problem of polynomial approximation



(a) Broadband π Pulse Shape (b) Experimental Offset Profile

Figure 1: Experimental excitation profiles of broadband π pulses. (a) The optimal broadband π pulse shape was derived by the multivariate pseudospectral method with the respective number of discretizations in time and frequency, $N = 36$ and $N_\omega = 12$, to cover the bandwidth $[-40, 40]$ kHz with limited rf amplitude $B_1(t) \leq 20$ kHz for all t and maximum duration $T = 120\mu$s. (b) The excitation profiles correspond to the optimal broadband pulse (red) and conventional hard pulse (black).

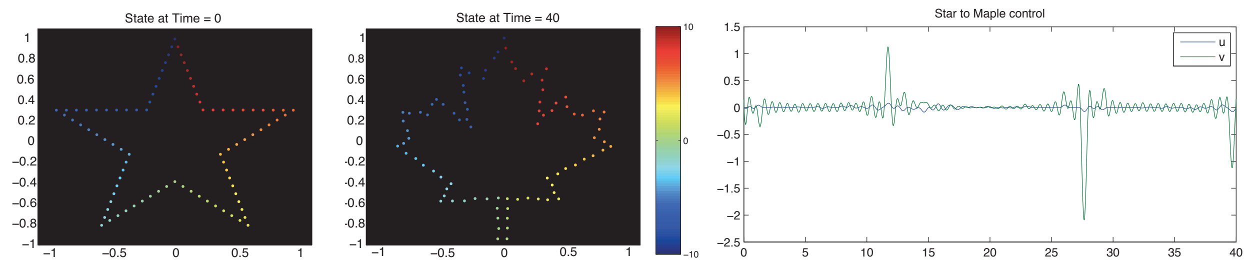


(a) Optimal Inversion Pulse (b) Adiabatic Inversion Pulse (c) Hard Inversion Pulse

Figure 2: HSQC spectra comparison. The ^{1}H-^{13}C correlated HSQC spectra of [^{13}C,^{15}N] GB1 sample using optimal inversion pulses (a), standard Bruker adiabatic inversion pulses (Crp60.0.5.20.1) (b), and conventional hard inversions (c). Spectra on the left of each pair were recorded when the ^{13}C-inversion pulses were on resonance (at 50 ppm), while the spectra on the right were recorded when the ^{13}C-inversion pulses were 31 kHz (at -200 ppm) off resonance to the up-field.

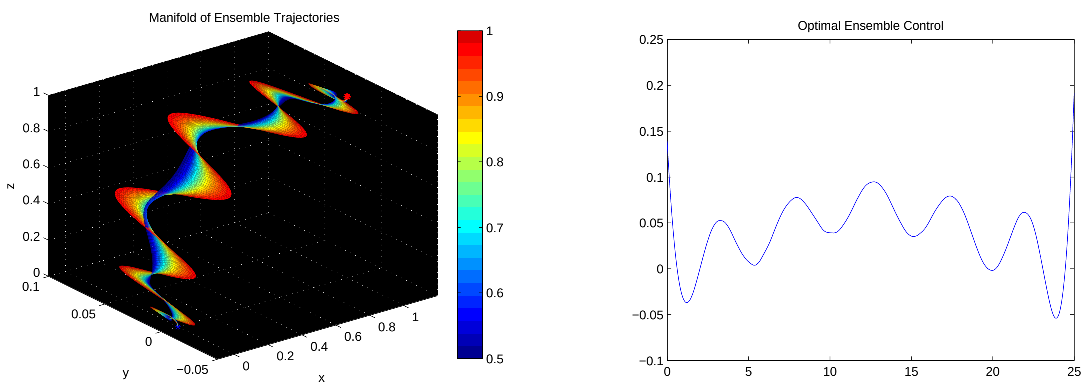
proposed in our previous work [3, 32], we developed a unified computational method for optimal pulse design in quantum control based on multidimensional pseudospectral approximations, by which a continuous-time optimal control problem of pulse design is discretized to a constrained nonlinear optimization problem using multivariate interpolating polynomials [6, 10]. This is the first work introducing pseudospectral methods to the quantum pulse design community.

Applications to Protein NMR Spectroscopy: Recently, in collaboration with Harvard Medical School, we have designed optimal broadband excitation ($\pi/2$) and inversion (π) pulses for protein NMR spectroscopy using this newly developed method. These broadband pulses have been experimentally implemented, yielding a significant sensitivity enhancement over the conventional hard pulse and adiabatic pulse while requiring a much shorter duration and lower energy [6]. The optimal pulse shape and the corresponding experimental excitation profile of the broadband inversion pulse are shown in Figure 1(a) and 1(b), respectively. The excitation profile was recorded with resonance offset ranging from -60 kHz to 60 kHz in steps of 2 kHz and showed that our opti-



(a) Ensemble State Transfer (b) Optimal Ensemble Control

Figure 3: Optimal control of an ensemble of harmonic oscillators as in (3). An ensemble of harmonic oscillators is steered (a) from the shape of a star to the shape of a maple leaf. The color indicates the natural frequency of the samples, where red and blue denote $\omega = 10$ and $\omega = -10$, respectively. (b) displays the ensemble control that accomplishes the desired transfer.



(a) Manifold of Ensemble Trajectories (b) Optimal Ensemble Control Law

Figure 4: Frictionless quantum transport of atoms. (a) An ensemble of atoms with the frequencies $\omega \in [0.5, 1]$ is transported from the initial state $(0, 0, 0)'$ to the target state $(1, 0, 1)'$. (b) The ensemble control law that accomplishes the desired transport is computed using the SVD method described in Section 2.2.

mal pulse has a noticeably higher average excitation profile over the designed bandwidth $[-40, 40]$ kHz than the conventional hard pulse. The two-dimensional spectra in Figure 2 illustrate a significant sensitivity enhancement over a conventional hard pulse and adiabatic pulse while requiring a much shorter duration - approximately a 20 times sensitivity enhancement over adiabatic pulses with a much shorter duration (120 μs versus 500 μs) [6]. In addition, this pseudospectral method can easily be modified to solve problems with other objectives, such as minimum-energy and time-optimal pulses, and requires much less computational power and time than state-of-the-art numerical methods for pulse design in NMR and MRI [6], such as the GRAPE algorithm [35] and the Krotov method [36].

Convergence of the Multidimensional Pseudospectral Method: We have, moreover, studied the convergence properties of this multivariate pseudospectral method for optimal ensemble control in Sobolev space, and it has been shown that given appropriate regularity conditions on the system dynamics and the control function, a sequence of optimal solutions to the discretized problem converges to an optimal solution of the original continuous-time optimal control problem [12, 20].

2.2 A Direct SVD Algorithm for Optimal Ensemble Control Synthesis for Linear Systems

As described in Section 1.1, the ensemble controllability conditions for time-varying linear systems as in (1) are characterized by the singular values and the corresponding singular functions of the linear operator (2) that governs the system dynamics. This new finding led us to develop an optimization-free computational algorithm based on the singular value decomposition (SVD) for the synthesis of optimal ensemble control laws for such linear ensemble systems [26]. The idea is to approximate the action of the compact operator L as in (2) on a function $u \in L_2^m[0,T]$ by a matrix acting on an appropriate vector of sampled values of u.

This SVD based algorithm, for example, has been successfully used to design optimal controls that steer the ensemble system (1) between any desired state configurations. A canonical example is to control an ensemble of harmonic oscillators,

$$\frac{d}{dt}\begin{bmatrix} x_1(t,\omega) \\ x_2(t,\omega) \end{bmatrix} = \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix}\begin{bmatrix} x_1(t,\omega) \\ x_2(t,\omega) \end{bmatrix} + \begin{bmatrix} u(t) \\ v(t) \end{bmatrix}, \tag{3}$$

with a variation, or uncertainty, in their frequencies, $\omega \in [\omega_1, \omega_2] \subset \mathbb{R}$. Figure 3 displays initial and final configurations between which the ensemble system (3) with $\omega \in [-10, 10]$ is transferred by the indicated optimal controls. Figure 4 illustrates the minimum-energy frictionless quantum transport of atoms with a variation in their frequencies using a harmonic trap [26, 17]. It is shown that the optimal ensemble control law displayed in Figure 4(b) is able to compensate for the variation in the frequency and achieve the desired transport. Furthermore, an iterative procedure based on this SVD method was developed for optimal control synthesis for bilinear ensemble systems [29].

3 Minimum-Time Frictionless Atom Cooling

Adiabatic processes are ubiquitous in cold atom physics, nuclear magnetic resonance, optics and other fields [37, 38, 39]. Although useful for preparing states robustly with respect to perturbations, these processes may become impractical due to their long duration. This has prompted a surge of theoretical and experimental activities to find shortcuts to adiabaticity in quantum systems. Such a task can be formulated as time-optimal control of quantum dynamics. We investigated several optimal control problems motivated by promising applications in quantum optics and coherent spectroscopy. These include time-optimal control of frictionless atom cooling in harmonic traps [5], which is a core of modern quantum technology [40, 41, 42]; frictionless decompression in minimum time of Bose-Einstein condensates [13], which is a workhorse for atomic physics experiments; and constrained minimum-energy control for dissipative spin systems [4]. We solved these optimal control problems analytically and verified the results with a pseudospectral method.

Personnel Supported

Jr-Shin Li, Principal Investigator

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Ji Qi, Current Graduate Student

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Publications During the Grant Period

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Peer-Reviewed Articles

1. D. Stefanatos and J.-S. Li, "Minimum-Time Quantum Transport with Bounded Trap Velocity", *IEEE Transactions on Automatic Control* (accepted).
2. A. Zlotnik, Y. Chen, I. Z. Kiss, H.-A. Tanaka, and J.-S. Li, "Optimal Waveform for Fast Entrainment of Weakly Forced Nonlinear Oscillators", *Physical Review Letters* (in press).
3. J.-S. Li, I. Dasanayake, and J. Ruths, "Control and Synchronization of Neuron Ensembles", *IEEE Transactions on Automatic Control* (in press).
4. D. Stefanatos and J.-S. Li, "Frictionless Decompression in Minimum Time of Bose-Einstein Condensates in the Thomas-Fermi Regime", *Physical Review A*, Vol. 86, 063602, 2012.
5. A. Zlotnik and J.-S. Li, "Optimal Entrainment of Neural Oscillator Ensembles", *Journal of Neural Engineering*, Vol. 9, 046015, 2012.
6. J. Ruths and J.-S. Li, "Optimal Control of Inhomogeneous Ensembles", *IEEE Transactions on Automatic Control: Special Issue on Control of Quantum Mechanical Systems*, Vol. 57, No. 8, pp. 2021-2032, 2012.
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15. D. Stefanatos and J.-S. Li, “Constrained Minimum-Energy Optimal Control of the Dissipative Bloch Equations”, *Systems & Control Letters*, Vol. 59, pp. 601-607, 2010.

Peer-Reviewed Proceedings

1. A. Zlotnik and J.-S. Li, “Iterative Ensemble Control Synthesis for Bilinear Systems”, *51st IEEE Conference on Decision and Control*, Maui, Hawaii, Dec., 2012.
2. D. Stefanatos and J.-S. Li, “Time-Optimal Adiabatic-Like Expansion of Bose-Einstein Condensates”, *51st IEEE Conference on Decision and Control*, Maui, Hawaii, Dec., 2012.
3. D. Stefanatos and J.-S. Li, “Time-Optimal Frictionless Atom Cooling in Harmonic Traps”, *51st IEEE Conference on Decision and Control*, Maui, Hawaii, Dec., 2012.
4. I. Dasanayake and J.-S. Li, “Charge-Balanced Time-Optimal Control for Spiking Neuron Oscillators”, *51st IEEE Conference on Decision and Control*, Maui, Hawaii, Dec., 2012.
5. A. Zlotnik and J.-S. Li, “The Synthesis of Optimal Ensemble Controls for Linear Systems using the Singular Value Decomposition”, *American Control Conference*, Montreal, Canada, Jun., 2012.
6. D. Stefanatos and J.-S. Li, “The Role of Singular Control in Frictionless Atom Cooling in a Harmonic Trapping Potential”, *American Control Conference*, Montreal, Canada, Jun., 2012.
7. P.-L. Liu, J.-S. Li, and T.-J. Tarn, “Quantum Multi-Channel Decoupling”, *The 10th World Congress on Intelligent Control and Automation*, Beijing, China, Jul., 2012 (Best Paper Award).
8. I. Dasanayake and J.-S. Li, “Constrained Minimum-Power Control of Spiking Neuron Oscillators”, *50th IEEE Conference on Decision and Control*, Orlando, Florida, Dec., 2011.
9. J. Ruths, A. Zlotnik, and J.-S. Li, “Convergence of a Pseudospectral Method for Optimal Control of Complex Dynamical Systems”, *50th IEEE Conference on Decision and Control*, Orlando, Florida, Dec., 2011.

10. A. Zlotnik and J.-S. Li, "Optimal Asymptotic Entrainment of Phase-Reduced Oscillators", *2011 ASME Dynamic Systems and Control Conference*, Arlington, Virginia, Oct., 2011.
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12. I. Dasanayake, I. Naqa, and J.-S. Li, "Constrained Kalman Filtering for IMRT Optimization", *49th IEEE Conference on Decision and Control*, Atlanta, Georgia, Dec., 2010.
13. J.-S. Li, "Control of a Network of Spiking Neurons", *8th IFAC Symposium on Nonlinear Control Systems*, Bologna, Italy, Sep., 2010.

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1. J. Ruths, "Optimal Control of Inhomogeneous Ensembles", PhD Thesis, Washington University in St. Louis, 2011.
2. I. Dasanayake, "Optimal Control of Weakly Forced Nonlinear Oscillators", PhD Thesis, Washington University in St. Louis, 2013.

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